

# Lattice-Gas Simulations of Ternary Amphiphilic Fluid Flow in Porous Media \*

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We develop our existing two-dimensional lattice gas model to simulate the flow of single phase, binary immiscible and ternary amphiphilic fluids. This involves the inclusion of fixed obstacles on the lattice, together with the inclusion of “no-slip” boundary conditions. Here we report on preliminary applications of this model to the flow of such fluids within model porous media. We also construct fluid invasion boundary conditions, and the effects of invading aqueous solutions of surfactant on oil-saturated rock during imbibition and drainage are described.

## I. INTRODUCTION

The lattice gas automaton (LGA) model introduced by Boghosian, Coveney and Emerton [1] has been used to investigate a variety of amphiphilic phenomena including the growth kinetics of binary immiscible fluid and ternary microemulsion systems [2,3], the effect of shear on ternary systems [4] and self-reproducing micelles [5]. In this article we describe the developments that have been made to allow invasive flow within a porous medium to be studied using this model. These developments open up a large area to possible investigation and we shall only give a very brief overview of the work done to date. We emphasise that the results presented here are preliminary and that considerably more work is needed in this area; much of this is currently in progress.

## II. DEVELOPMENT OF THE MODEL

For a discussion of the original model, the reader is referred to Boghosian, Coveney and Emerton [1]. In the general case, the model admits the presence of three different species of particle, which are distinguished by their “colors” (red for oil, blue for water, and green for surfactant). The modifications to the model

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which are made in this paper fall into two categories: the implementation of bulk flow and the alteration of boundary conditions.

The study of bulk flow had previously been limited to the case of linear shear flow [4]. The new techniques we have implemented use a similar method to that of Olson and Rothman [6,7]: momentum is added at random sites throughout the fluid. As the particles are situated on a discrete triangular (FHP) lattice with six lattice vectors, the change in momentum at any given site may be quite large although the global effect is small. This is not unreasonable as the propagation and collision steps of the model (which impart viscosity to the fluids) distribute this momentum in a relatively short time. However, while Olson and Rothman manipulate each particle separately, in our code use is made of the pre-existing look-up tables for the maximum and minimum momentum in the y-direction (vertical) that were used for shear flow [4]. Previously, sites on opposite sides of the lattice were looped over in a stochastic manner and their momentum updated until the shear boundary condition was met. For bulk flow the *entire* lattice is looped over and either:

1. enough sites are updated for the total average momentum of the particles to be equal to a set value; this is called the implementation of a ‘pressure gradient’. This is not a true pressure gradient, since pressure is proportional to the density of the fluid. This is the flow implementation used throughout this article;

or

1. enough sites are updated so that the total additional momentum applied to the system of particles in each timestep is equal to a constant, thus simulating bulk flow under gravity, i.e. *buoyancy* effects.

To model flow through porous rock, a channel or any other obstacle structure, a no-slip boundary condition needs to be set up at the interface between the particles and a general obstacle matrix. The no-slip boundary condition applied to a Navier-Stokes fluid corresponds to a ‘bounce-back’ step in the lattice-gas model [8,9].

There are three components to the successful implementation of a realistic no-slip boundary condition [8]:

1. First, in the initial set-up of the lattice, the obstacle matrix has to be cleared of all particles. It will then remain so for all time.
2. Second, a simple “bounce-back” operation is carried out, in which a particle colliding with an obstacle has its momentum reversed in sign.
3. Finally, obstacles may be given a specified color charge, thus assigning certain wettabilities to the simulated rock species.

In the present paper, which presents purely preliminary results, only the effects of an obstacle site color density of  $\pm 7$  are reported (equivalent to that for a site *full* of either red or blue particles), but it is possible to alter the ‘strength’ of each site’s wettability to any integer value between these values.

To allow invasive flows to be studied, the model maintains horizontal periodic boundary conditions, but is no longer periodic in the vertical (forced) direction. We must concern ourselves with particles that stray off the top and bottom of the lattice. Conserving the mass of the particles on the lattice imposes restrictions on the fate of these particles: we cannot, for example, arbitrarily add particles to the base of the lattice since this violates the conservation of mass. Hence we are forced to wrap the particles from top to bottom and *vice versa*, but if an *oil* particle propagates off the top of the lattice, then on the subsequent timestep we re-introduce this particle as a *water* particle at the base of the lattice moving in the same direction as when it left the lattice. This satisfies the mass conservation law and also imitates the physical process under study. An extension of this is required if surfactant is present in the invading phase.

A further modification is required to convince the particles on the top and bottom rows of the lattice that they are below and above infinite columns of oil and water respectively. This is done by adding two extra “invisible” rows which affect the collisions on the top and bottom rows, but which play no part in particle propagation.

Note that in order to incorporate the most general form of interaction energy within the model system, a set of coupling constants  $\alpha, \mu, \epsilon, \zeta$ , are introduced, in terms of which the total interaction energy can be written as

$$\Delta H_{\text{int}} = \alpha \Delta H_{\text{cc}} + \mu \Delta H_{\text{cd}} + \epsilon \Delta H_{\text{dc}} + \zeta \Delta H_{\text{dd}}. \quad (1)$$

These terms correspond, respectively, to the relative immiscibility of oil and water, the tendency of surrounding dipoles to bend round oil or water particles and clusters, the propensity of surfactant molecules to align across oil-water interfaces and a contribution from pairwise (alignment) interactions between surfactants. In this report, as in previous studies [1–4]  $\beta = 1.0$  and the coupling constants are given the values

$$\begin{aligned} \alpha &= 1.0 \\ \mu &= 0.001 \\ \epsilon &= 8.0 \\ \zeta &= 0.005, \end{aligned}$$

strongly encouraging surfactant molecules to accumulate at oil-water interfaces while maintaining the normal oil-water immiscible behavior.

Different porous media have been constructed. The random location of obstacles (spheres or squares) is the method most commonly used to construct an artificial porous medium. In the present work, we have used a novel modification of this technique which allows one to control the size and connectivity of the obstacle matrix without introducing artificial symmetries. In this approach, an initial simulation is run leading to a microemulsion phase (droplet or sponge). Droplets of, say, oil are formed and grow with time. When their size reaches some desired value, the positions of these oil particles are stored as obstacle sites for later simulations. Suitable modification of the initial conditions (reduced densities, flow conditions and so on) produces a wide range of porous media for subsequent study.

### III. DARCY'S LAW

Darcy's Law relates the flux of a *single phase* fluid through a porous medium to the gradient of pressure across the medium. Mathematically, Darcy's law can be written:

$$u = -\frac{k}{\mu} X \quad (2)$$

where the constant  $k$  is the *permeability* of the medium,  $\mu$  is the dynamic viscosity and  $X = -\nabla P + \rho g$  is the fluid forcing (pressure gradient plus gravitational force density). This relation was verified using our code on different porous media. The results presented in this section are obtained using the porous medium shown in Fig. 1.

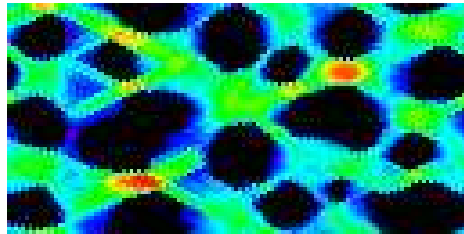


FIG. 1. The porous medium used in the simulation discussed in section 3, together with a coloured velocity profile for a single component fluid flow.

### A. Binary Immiscible Flow

There is no widely accepted extension of Eq. (2) which deals with the case of two-phase or multiphase flows within porous media. It is frequently asserted that Eq. (2) generalises to two or more similar but completely uncoupled equations, in which the *relative permeabilities* make an appearance. Experimental [10] and numerical [11,12] work has suggested an extension of Eq. (2) including coupling terms between the two fluids:

$$\begin{pmatrix} u_w \\ u_n \end{pmatrix} = k \begin{pmatrix} \kappa_{ww} & \kappa_{wn} \\ \kappa_{nw} & \kappa_{nn} \end{pmatrix} \begin{pmatrix} F_w \\ F_n \end{pmatrix}, \quad (3)$$

where the subscript ‘w’ indicates a ‘wetting’ phase and the subscript ‘n’ indicates a ‘non-wetting’ phase. The new transport coefficients  $\kappa_{ij}$  are *relative permeabilities* (diagonal terms) and coupling coefficients (off-diagonal terms). In general these  $\kappa_{ij}$  will depend on the viscosity of each fluid and the composition of the mixture. The force acting on particles in Eq. (2) has been replaced by the gravitational force, as used in the previously described simulations. This technique is closely related to several other implementation methods [6,7].

Much has been made of the reciprocity of the  $\kappa_{wn}$  and  $\kappa_{nw}$  coupling coefficients, and its possible relationship with Onsager’s reciprocity relations in linear non-equilibrium thermodynamics [13,14]. Some theoretical work has been done on this subject for the linear regime [15], but no explanation exists for the generally nonlinear behavior displayed in lattice-gas models. There is also a quite surprising lack of experimental data available by means of which to resolve this issue.

Fig. 2 shows the results of measurements made on the flow of wetting and non-wetting phases when either of these phases are forced in a water wetting porous medium; the graphs describe the relative permeabilities (seen as the supposedly constant gradients of the curves) from the matrix of Eq. (3) for reduced densities of oil and water equal to  $\rho_i = 0.25$ . Each data point on a plot represents the result from a single run, averaged over 20,000 time steps for a  $64 \times 128$  lattice. In this binary immiscible case, the maximum ‘pressure’ that can be applied to the system is approximately 0.025 momentum units per lattice site (the ‘gravity’ condition is used). The relative permeabilities (diagonal elements of the matrix in Eq. (3)) appear to be constant over most ‘pressures’, with a least-squares fit plotted on the figures.

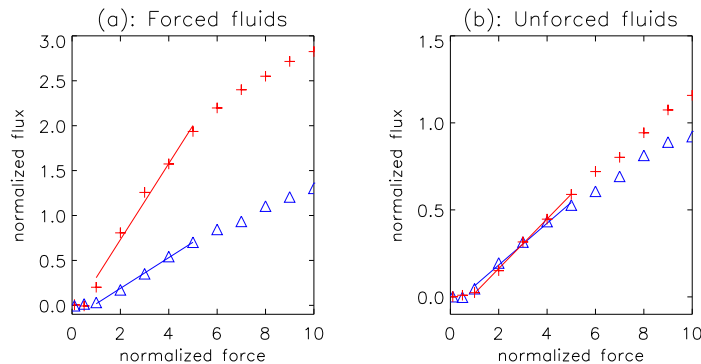


FIG. 2. Darcy’s law behavior for binary immiscible fluids. Triangles correspond to the response of water and crosses to the response of oil. The normalized flux and force are defined in the same way as by Olson and Rothman, for a forcing of 0.001 per lattice site. The lines represent least-squares fits to the data.

As in the three-dimensional simulations of Olson and Rothman [6], when the fluids are forced the curve pertaining to the non-wetting fluid, Fig. 2(a), shows capillary effects at low forcing levels. Droplets of the non-wetting fluid are trapped in the medium, resulting in a disconnected phase. Nevertheless, the wetting fluid also exhibits a nonlinear behavior in the same regime. This is because, in the 2D porous medium, the obstacle matrix is not continuous so a certain ‘pressure’ is required before the wetting fluid can break through its surface tension and flow. However, the non-wetting fluid is ‘lubricated’ by the wetting fluid,

causing it to flow readily. This ‘lubrication’ is mainly responsible for the different slopes, or different relative permeabilities, for the two phases. The differences in the response of water and oil when they are forced arise directly from the wettability of the rock versus water.

From inspection of Fig. 2(b) it is clear that the definition of the coupling coefficients as constants is approximately valid, for pressure gradients above a capillary threshold. Moreover, it can be seen that the responses of the unforced fluids are roughly symmetric. The results are thus consistent with Onsager reciprocity. At high ‘pressures’ the water ‘slides’ up around the obstacles and around the oil drops, imposing a slowly increasing force on the non-wetting phase.

It is important to notice the various scales on the flow axes: the coupling of the two phases is significant. This coupling is the consequence of the large amount of fluid-fluid interface, and is related to the average pore size in the porous medium. Taking the relative permeabilities to be constant over all ‘pressures’ above the capillary threshold, their calculated values are  $\kappa_{ww} = 0.17 \pm 0.0007$  and  $\kappa_{nn} = 0.42 \pm 0.003$ . The values for the coupling coefficients are  $\kappa_{wn} = 0.14 \pm 0.0009$  and  $\kappa_{nw} = 0.12 \pm 0.0003$ .

### B. Ternary Amphiphilic Flow

Fig. 3 shows the results of measurements made on the flow of wetting and non-wetting phases when either of these phases are forced (in the same water-wetting porous medium). The reduced densities of wetting and non-wetting fluids was 0.2 and the simulations were performed at the same total density as before. These results are qualitatively similar to those obtained in the binary immiscible case. However, some differences do exist:

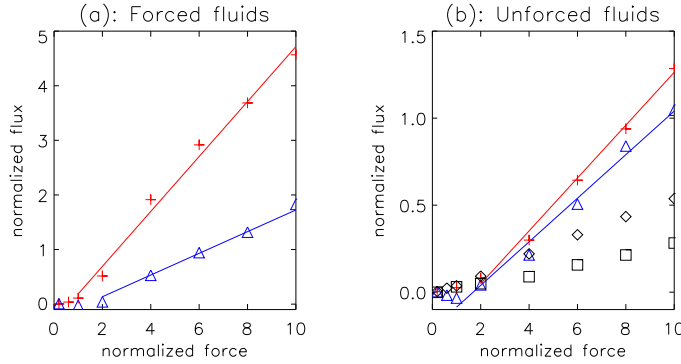


FIG. 3. Darcy’s law behavior of ternary amphiphilic fluids. Triangles correspond to the response of water and crosses to the response of oil. Squares and diamonds correspond to the response of surfactant when oil or water is forced respectively. The normalized flux and force are defined in the same way as by Olson and Rothman, for a forcing of 0.0005 per lattice site.

1. Firstly the values for the relative permeabilities in the ternary case are  $\kappa_{ww} = 0.21 \pm 0.005$  and  $\kappa_{nn} = 0.51 \pm 0.084$ . The values for the coupling coefficients are  $\kappa_{wn} = 0.15 \pm 0.004$  and  $\kappa_{nw} = 0.12 \pm 0.005$ . The marked change in  $\kappa_{ww}$  and  $\kappa_{nn}$  is due to a lowering in the surface tension between the oil and water phases now that surfactant is present at the interface; the water then flows more easily through the large channels within which the non-wetting oil would otherwise sit.
2. The flux of the fluids when they are not forced is roughly the same as in the binary case. Their responses are still essentially symmetric. The response of surfactant is also shown, which varies linearly with the forcing level.
3. The capillary threshold is lower than in the binary case (here equal to 0.0005). This can be explained by the reduction in surface tension when surfactant is present (oil can pass more easily through narrow channels).

#### IV. STUDY OF THE EFFECT OF SURFACTANT ON FLUID INVASION IN POROUS MEDIA

No lattice gas automaton model has previously investigated the effect of surfactant on an oil/water system undergoing invasive flow. We start from a porous medium filled with oil into which water invades; this invading phase may contain varying amounts of surfactant and the effect of this on oil production is studied qualitatively in this preliminary study. The obstacle matrix may also be given different wetting properties (oil-, water- or non-wetting). With water as the invading phase, the case with oil-wetting obstacles corresponds to drainage and that with water-wetting obstacles to imbibition. In the present model, only particles on lattice sites containing water are forced. Unlike previous non-invasive studies, the number of forcing particles on the lattice increases with time. Although this is taken into account in deciding the maximum forcing amplitude that can be applied, it can lead to spurious effects. When there is an insufficient quantity of water present, the water is “over-driven” and, for example, small droplets of water can detach from the bulk phase and are hence propelled into the oil. Moreover, the flow of surfactant particles is entirely dependent on the transfer of momentum from forced water particles. Thus, although a specified proportion of surfactant is placed on the bottom row of the lattice, some may fail to propagate into the bulk of the invading phase. Both of these features limit the preliminary study reported here to being a qualitative approach only. We plan to return in the future with a more quantitative study.

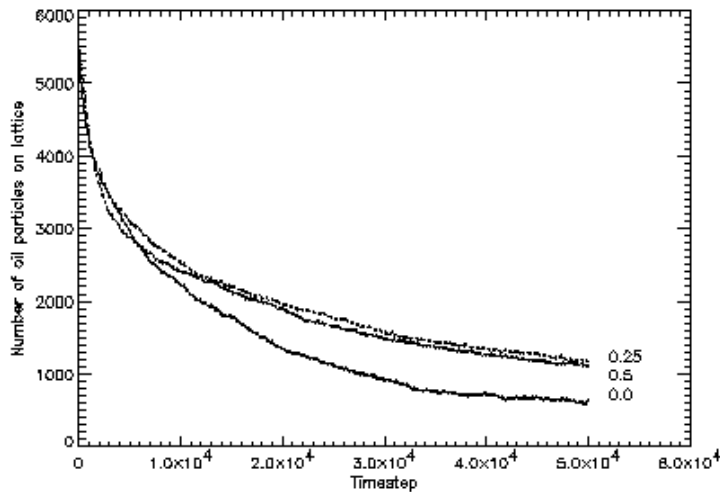


FIG. 4. Graph showing how the amount of oil on the lattice changes with time for drainage with different relative concentrations of surfactant.

The effect of aqueous surfactant concentration on oil production is investigated by tracking the amount of oil on the lattice as a function of time. We first consider the phenomenon of drainage (Fig. 4). More oil is expelled off the lattice if *no* surfactant is present. The difference between concentrations 0.25 and 0.5 is too small to allow any conclusions about their relative magnitudes to be drawn. A second study revealed a similar effect. (Both studies used a 64×64 lattice and a forcing amplitude of 0.010.)

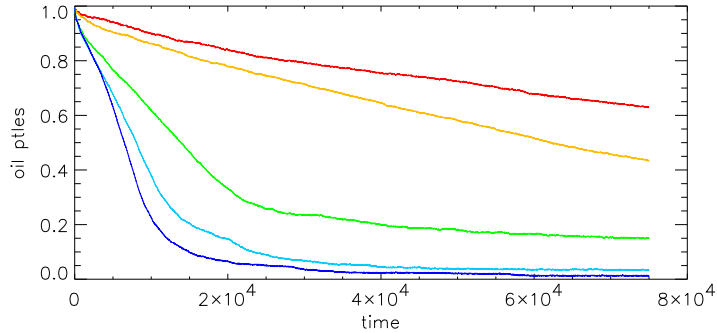


FIG. 5. Effect of the applied force in imbibition simulations. The different forcing levels (from top to bottom) are 0.0005, 0.001, 0.005, 0.01, 0.025

Now let us turn to the case of imbibition. The two imbibition investigations which we have performed in these preliminary investigations show quite marked variations. In one study, we found that the presence of surfactant improved the recovery of oil dramatically. However, a second study found that the presence of surfactant made little difference to this process. Each investigation used a different obstacle matrix in addition to other differences in the parameters used, all of which no doubt contribute to produce these differences. We believe that, although the behavior we have found so far is inconclusive, further more detailed investigations will produce interesting results from which more systematic conclusions may be drawn, and we plan to publish our findings in due course.

One expects that percolation plays a large role in the behavior of these systems [16]. Fig. 5 shows imbibition simulations for different driving forces. One can see that as the driving force increases, not only the time needed to reach the asymptotic behavior decreases but so does the residual oil saturation. Prior to percolation, the invading fluid (water) phase bodily drives oil off the lattice. The variation of the number of oil particles versus time is roughly linear. After the percolation threshold for water, the decrease of the number of oil particles is less pronounced. The end of oil percolation leads to the asymptotic regime (defining the residual oil saturation). This overall behavior depends on the driving force, the concentration of surfactant present (and obviously on the porous medium). For example, it is possible to envisage a scenario where the percolation channels are wide enough to sustain the flow of the invading phase and hence no further oil is driven from the lattice, leading to high residual oil saturation. The influence of percolation on this behavior is currently under investigation.

Fig. 6 shows four graphical snapshots of the system at the same timestep but with different configurations. Figs. 6 (a) and 6 (b) show drainage without and with surfactant present in the invading phase respectively. Figs. 6 (c) and 6 (d) are similar but show the case of imbibition. All are from timestep 8,000. These snapshots are intended to illustrate qualitative differences only.

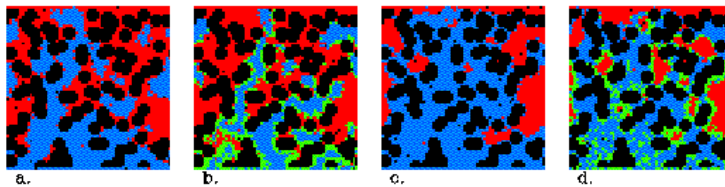


FIG. 6. Invasive flow of water in drainage and imbibition. The snapshots show different configurations at timestep 8,000: (a), (b) drainage without and with surfactant, respectively; (c),(d) imbibition without and with surfactant, respectively.

Figs. 6 (a) and 6 (b) suggest that the presence of surfactant permits the formation of stable percolating channels by the invading aqueous phase, leading to greater oil retention within the porous medium. Figs. 6 (c) and 6 (d), which are taken from the first of the two studies of imbibition mentioned above, suggest that, at least if there are relatively large voids in the porous medium, aqueous surfactant can break down and hence remove—by emulsification and/or micellization—the pockets of oil trapped within the rock. Nevertheless, the time scale over which such phenomena occur could slow down the oil production process. We emphasise again, however, that these are purely preliminary results valid in specific cases. Further work will be necessary before it is possible to establish whether any general conclusions can be drawn.

## V. DISCUSSION

We have described an extension of our hydrodynamic lattice-gas model to handle invasive flows within two-dimensional porous media. This has allowed us to investigate a generalization of Darcy’s law for multiphase flows, including effects due to the presence of surfactant. Invasion studies in porous media produced some interesting preliminary results, particularly in connection with the presence of surfactant within the invading phase. However, to permit a more complete and quantitative analysis, further developments and more detailed simulation studies are required; indeed, some of these are already underway. For example, one might consider devising alternative fluid forcing algorithms for improved handling of the flow of the invading phase; *inter alia*, as noted above, surfactant and water could be forced together. A more detailed investigation of the role of percolation is required. The reliability of our results would be enhanced by the use of larger lattices and increased statistical averaging. Throughout the work discussed here, both water-wetting and oil-wetting porous rock obstacles have been made maximally wetting. If the color charge on the obstacle sites were reduced, the phenomenological behavior could be expected to change significantly. These comments reflect the quandary faced when deciding what to investigate with this model. Considering merely invasive studies, there are evidently many important areas now open for investigation and many parameters which could be altered, although this report has only touched on a few of these. Not of least importance is the structure of the porous medium itself: one can expect significant changes in flow behavior in going from two to three dimensions. We hope to address more closely the real world using a three-dimensional version of our model [17] at some stage in the future. However, two-dimensional experimental systems exist for studying porous media flows—so-called “micromodels”—and we believe that there is already scope for a valuable dialogue between our simulations and experiments in this area [18].

## VI. CONCLUSION

The results on binary immiscible and ternary amphiphilic fluids show that the presence of surfactant, when either phase is forced, increases the flow of the forced phase. The relative permeabilities seem well behaved in both the binary immiscible and ternary amphiphilic fluids, while the coupling coefficients are more dependent on the actual geometry and dimensionality of the obstacle matrix. Moreover, the capillary threshold is lowered by the incorporation of amphiphilic particles.

The study of ternary amphiphilic invasion into a porous medium showed that the introduction of surfactant into the invading phase alters drainage and imbibition. Preliminary results have shown that the addition of surfactant seems to impair drainage. However, we cannot yet make any conclusive remarks about the effect of surfactant on imbibition.

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